Atomic Interface Design of Nanocomposites with Superior Shock Tolerance

Ruifeng Zhang, T-3;
Timothy C. Germann, T-1;
Jian Wang, MST-8;
Irene J. Beyerlein, T-3

A new empirical potential for a Cu/Nb system is developed that accurately captures deformation twinning in body-centered cubic (bcc) metals and the mechanical response of bimaterial incoherent Cu/Nb interfaces in the extreme conditions of shock compression. Using this potential, we demonstrate the important role of atomic interface structure on the dislocation-mediated plastic response of Cu/Nb nanolayered composites in shock compression. The activation barriers for the nucleation of dislocations from and the transmission of dislocations across an atomically flat interface are found to be substantially higher than those from an atomically faceted interface (that is, an interface comprised of a regular array of steps).

For next generation advanced materials, the scientific and technical demand has been increasing for a design such that the next generation advanced materials that can withstand extreme mechanical loadings, such as severe plastic deformation (SPD) and shock loading. Promising candidates are nanostructured composite materials with a high bimaterial interfacial content. In such nanomaterials, the atomic interface structure deviates significantly structurally and/or chemically from that of the bulk crystals that they join. Under extreme mechanical loadings, the interfaces can serve as a barrier to plastic flow, act as a source of dislocations, and accommodate deformation by rotation or sliding, etc. Different interfacial defect characteristics can alter the way the interface responds to extreme mechanical loadings.

To elucidate this unique structure-property relationship, a realistic atomistic simulation plays an important role in revealing how the interface responds to the mechanical loadings and interactions with dislocations. In our recent studies, we have focused our modeling efforts on the face-centered-cubic (fcc)-bcc nanocomposite (e.g., Cu/Nb nanolaminate composites) as a prototype system. We found that an obstacle for achieving realistic atomistic simulations in shock loading for bcc metals, such as Nb, and fcc-bcc binary systems, such as Cu-Nb, was the inaccuracy of existing potentials in the high-pressure regime. Current potentials lead to an artificial structural phase transformation under high pressure for bcc-Nb that disagrees with density functional theory (DFT) calculations and experiment observations. Thus, they are inappropriate for shock compression studies (Fig. 1) [1]. We discovered that the source of the problem was the existence of artificial minima in the high-pressure gamma surface. At 50 GPa, only the Ackland Finnis-Sinclair (FS) potential and force-matched embedded atom method (EAM) potentials can successfully capture the associated changes in the gamma surface predicted by DFT. Such findings set a foundation for reliable atomistic shock simulations that involve materials that are bcc or contain a bcc constituents, such as two-phase Cu-Nb composites. Using the elemental Ackland potential for Nb and Voter-Chen Cu potential, we developed a new Cu/Nb interatomic cross potential, which can accurately described both Cu/Nb interface structure and the high-pressure response of the Cu and Nb constituents.

Utilizing the newly constructed Cu/Nb potentials and non-equilibrium molecular dynamics (MD) simulations, we successfully revealed the dislocation processes underlying the pronounced effect of atomic interface structure on the plastic response of Cu/Nb nanolayered composites to shock compression [2,3], which was recently observed in experiments. Furthermore, we demonstrated that the critical shock pressures to nucleate and transmit dislocations across an atomically flat interface (e.g., KS interface) is substantially higher than those from a faceted interface (e.g., {112}KS interface) [2]. The reasons can be related to atomic-level interface dislocation characteristics that cause these two interfaces to nucleate, absorb, and transmit dislocations by significantly different mechanisms (Fig. 2). We have also studied the effect of layer thickness on the mechanisms of shock deformation. The study reveals an inverse size-dependence. We find enhanced shock resistance with decreasing layer thickness above a critical layer thickness, while below this thickness the shock resistance deterioriates with decreasing layer thickness due to the onset of large amounts of dislocation nucleation from the interfaces. These results will be presented in a forthcoming paper.

For more information, contact Irene J. Beyerlein at irene@lanl.gov.

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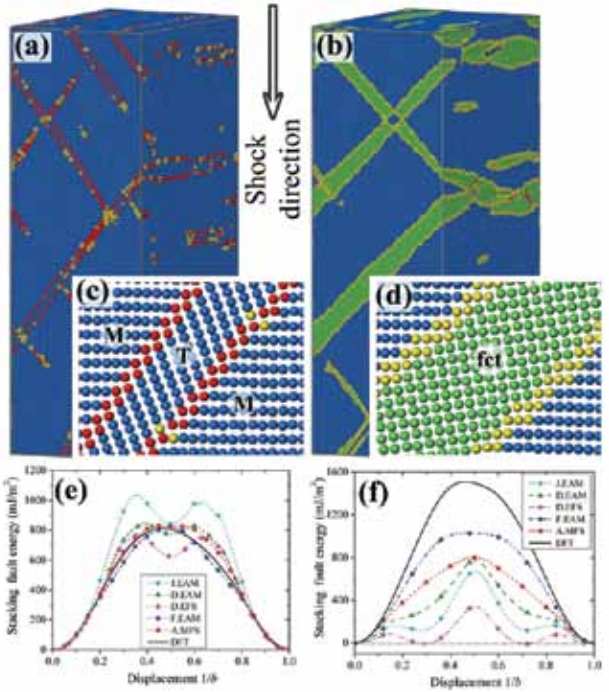

Fig. 1. Two types of structural changes that develop in an Nb single crystal under shock loading: (a) deformation twinning using the A.MFS potential and (b) bcc-fct phase transformation using the D.EAM potential, (c) a magnification of the twin structure, and (d) a magnification of the fct structure. The GSF curves on the {112} plane along the <111> direction at (e) zero hydrostatic pressure and (f) 50 GPa hydrostatic for the five empirical potentials and DFT. Local minima are found for the J.EAM, D.EAM, D.EFS potentials.

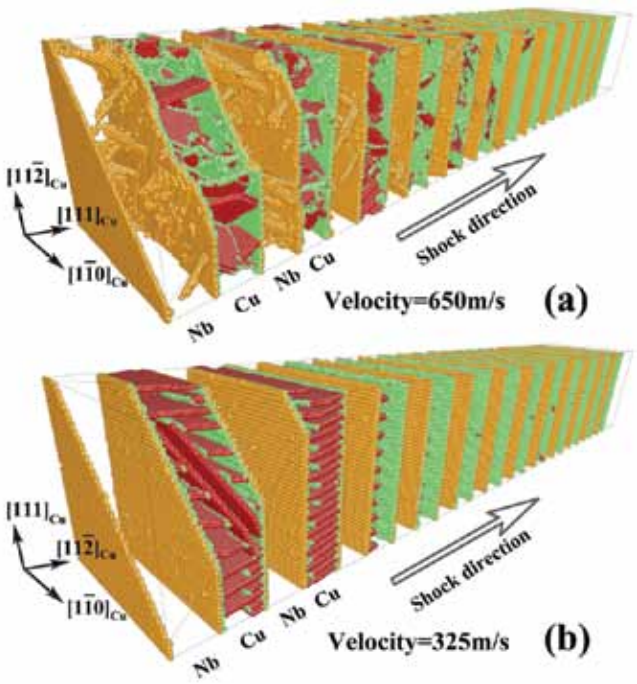

Fig. 2. Perspective view of shock-induced dislocation nucleation and transmission [2,3] from (a) flat KS interfaces at the piston speed of 650 m/s and (b) faceted {112}KS interfaces at up = 325 m/s during shock compression.

[1] Zhang R.F. et al., *Phil Mag Lett* **91**, 731 (2011).

[2] Zhang R.F. et al., *Scripta Mater*, in press; doi: http://dx.doi.org/10.1016/j.scriptamat.2012.09.022 (2012).

[3] Zhang R.F. et al., *AIP Conf Proc* **1426**, 1251 (2012).